Alloy scattering of substitutional carbon in silicon: A first principles approach

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- Substitutional carbon in silicon
- Scattering theory in a nutshell
- Density functional theory
- Supercells calculations
- Formulation of the method
- Results

- Strain compensation in SiGe/Si heterostructures
- Suppression of dopant diffusion during growth

What effect will substitutional carbon have on the mobility?

- Require knowledge of carrier scattering

Probability of transitions between states found from a transition matrix.

$$\langle \psi_{\mathbf{k}'} | \Delta V | \psi_{\mathbf{k}} \rangle$$

Matrix element formed from the inner product of the two states with the change in potential ΔV.

Scattering rate found from matrix element using Fermi's Golden Rule.

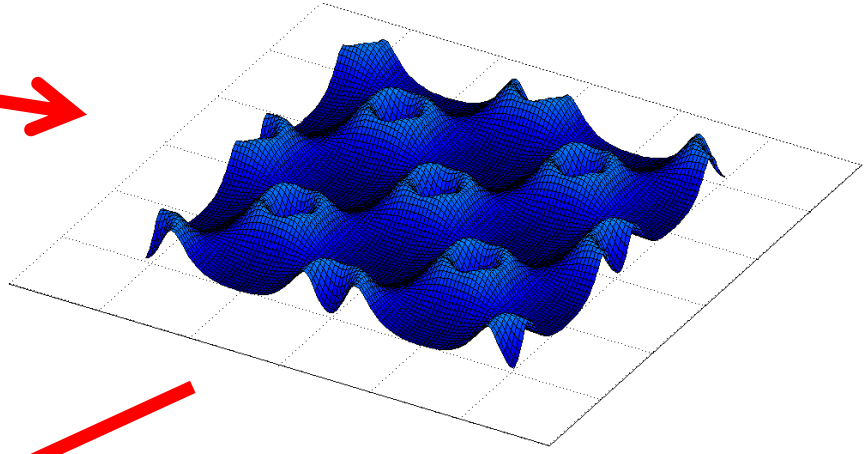
$$\frac{1}{\tau(E)} = \frac{2\pi}{\hbar} \left| \langle \psi_{\mathbf{k}'} | \Delta V | \psi_{\mathbf{k}} \rangle \right|^2 D(E_{\mathbf{k}'})$$

($\tau(E)$ is the 'relaxation time' and $D(E)$ is the density of final states)

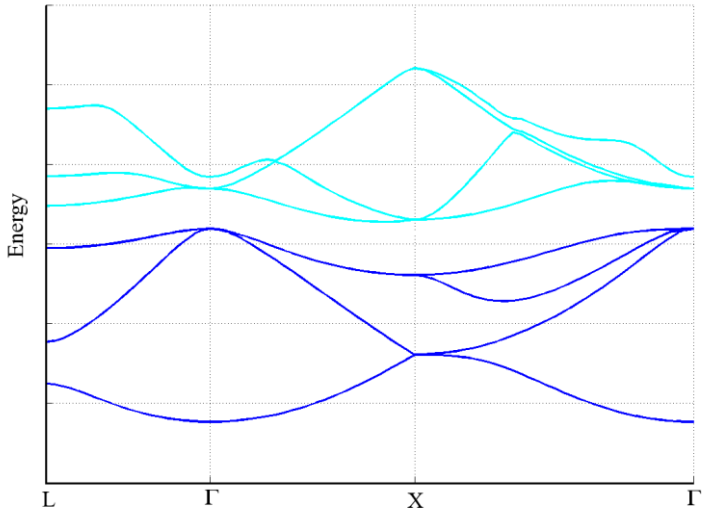
Density functional theory

Self consistent field calculations

Ground state density (+ potential)



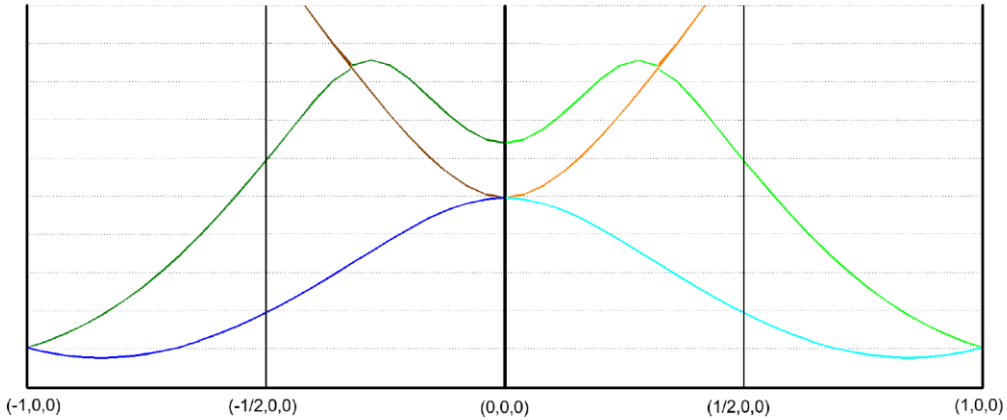
Single-particle solution



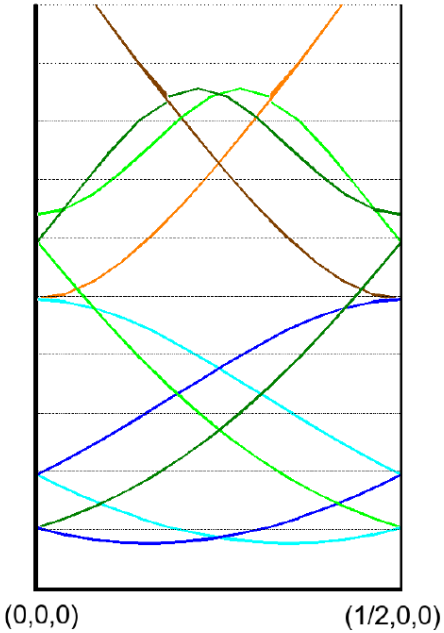
Band structure eigenvectors and eigenvalues

Post-processing of wavefunctions…

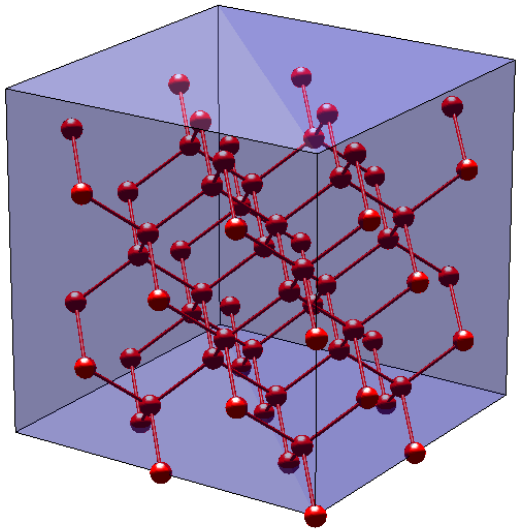
Primitive cell Brillouin zone
(energy v wavevector)



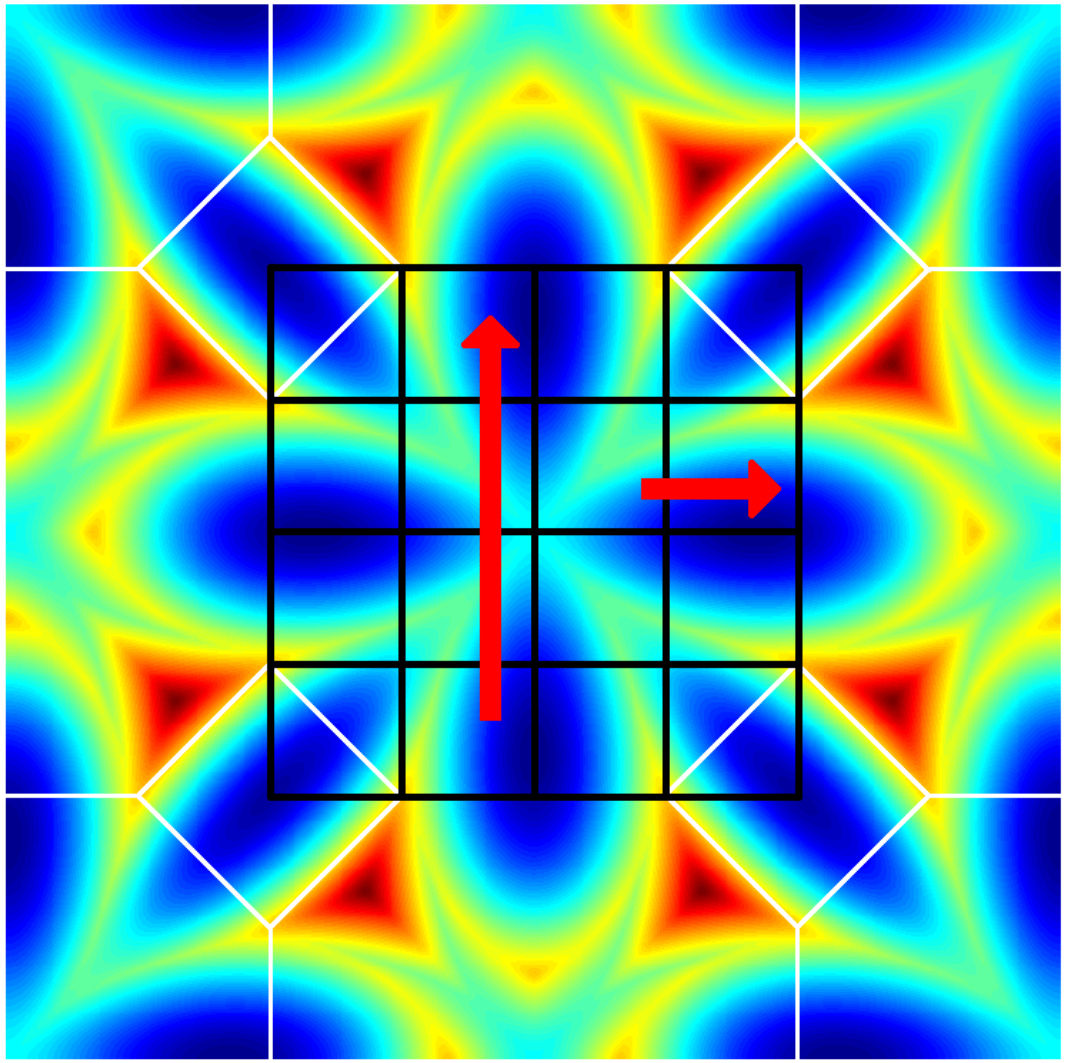
Folded into supercell BZ



64 atom supercell



Supercells calculations – Brillouin zone folding



64 atom supercell BZ (black squares)

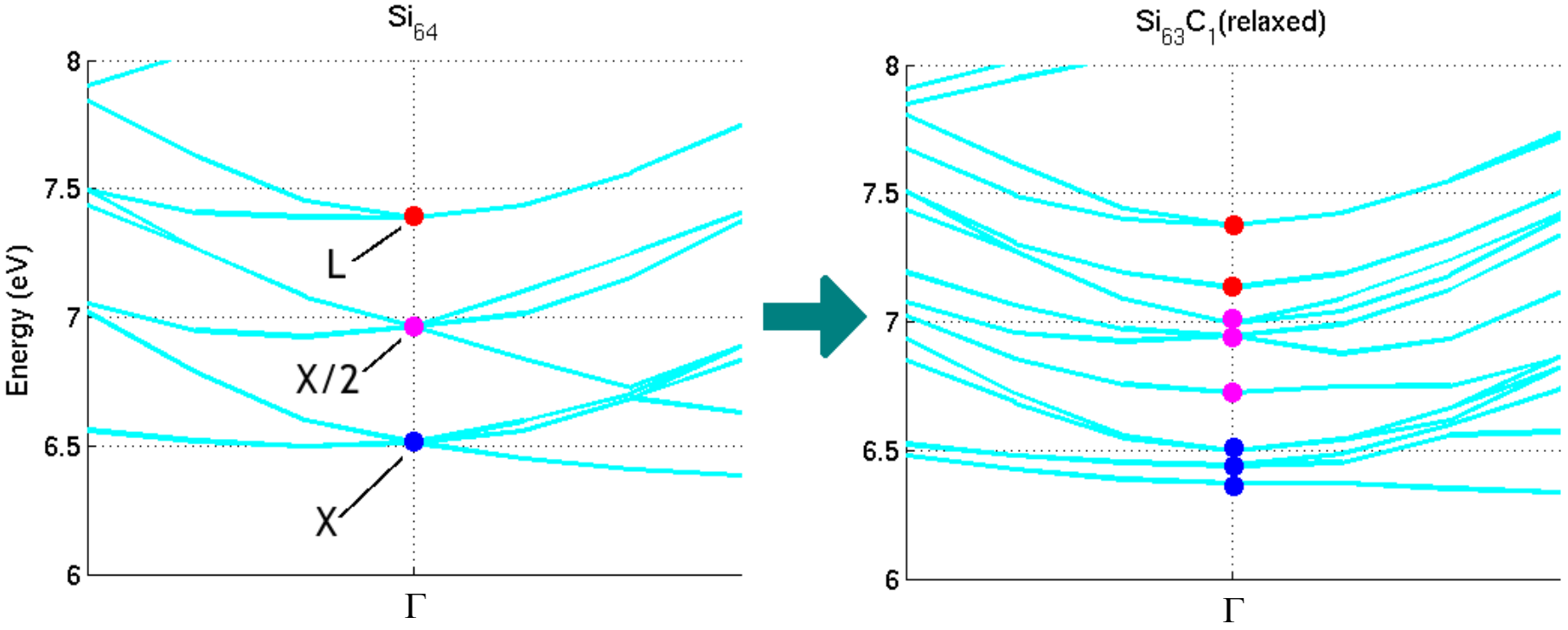
mapped into the primitive cell BZ (white lines)

showing example 64 atom reciprocal lattice vectors (red arrows).

Supercell can be used to represent scattering in the primitive BZ by a reciprocal lattice vector.

Replace an Si atom with a C atom

- Eigenvalues now perturbed
- New eigenstates considered as a mixture of the unperturbed states



Example: Γ point in a 64-atom supercell

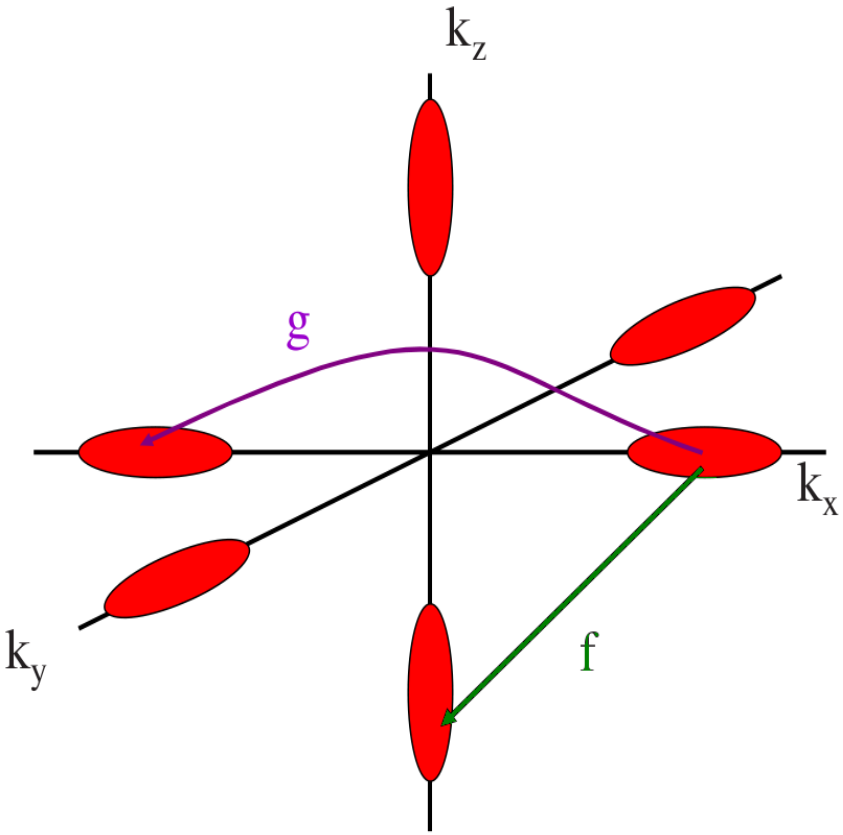
Constructing a Bloch basis for the new Hamiltonian

- Construct perturbed Hamiltonian (with C atom) using a basis of primitive Bloch functions (for each reciprocal lattice vector)
- The off-diagonal elements then give the transition matrix elements (for non-zero momentum change)

$$\langle \psi_i | \Delta V | \psi_j \rangle \delta_{ij} = \langle \psi_i | H - H_0 | \psi_j \rangle \delta_{ij}$$

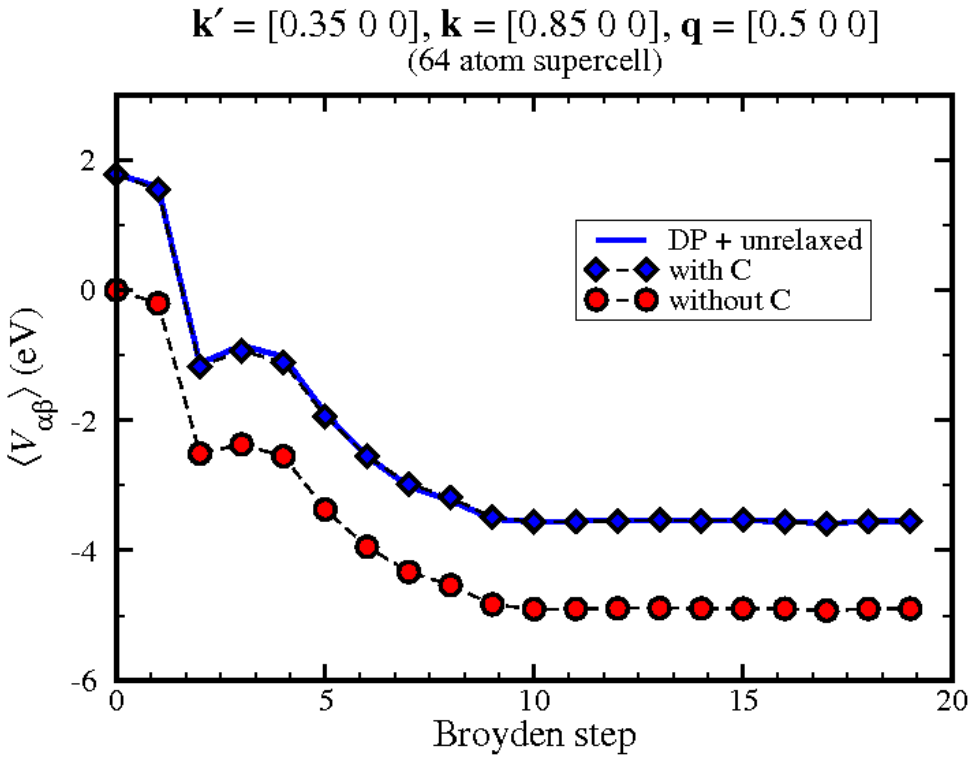
- Important note: because the zero of a pseudopotential is arbitrary, the diagonal matrix elements of H will include an unknown shift in energy between the C and Si potentials.
- Matrix elements constructed from wavefunction coefficients and eigenvalues of primitive and perturbed systems
- Non-diagonal elements do not involve primitive eigenvalues
- Details to be published…

- Intravalley
- Intervalley
  - f-type
  - g-type

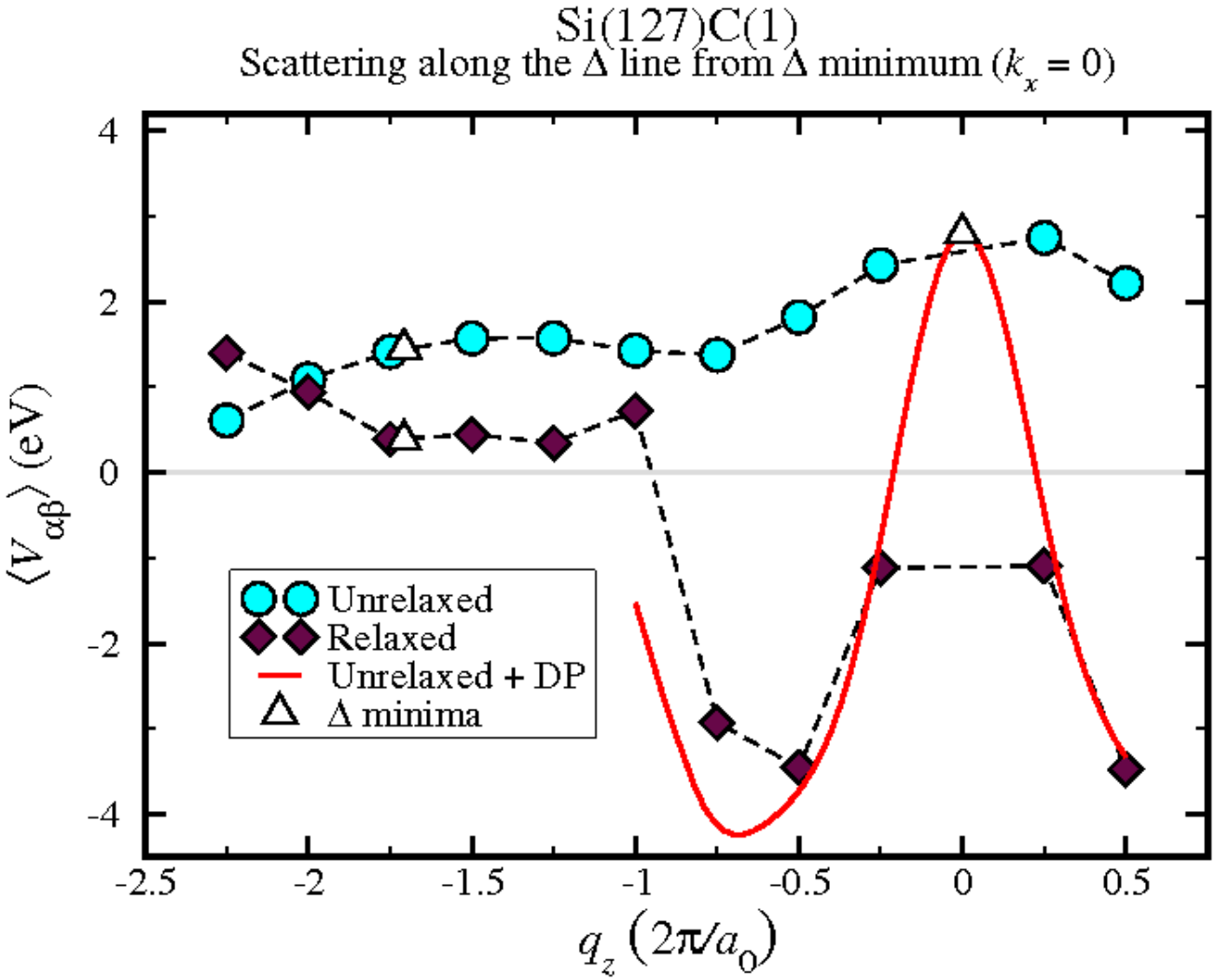


g and *f*-type intervalley scattering
[image from *Phys. Rev. B*, **78**, 35202 (2008)]

- Ionic positions are relaxed to lowest energy configuration
- Scattering can be decomposed into two parts
  - Chemical part
  - Deformation potential part

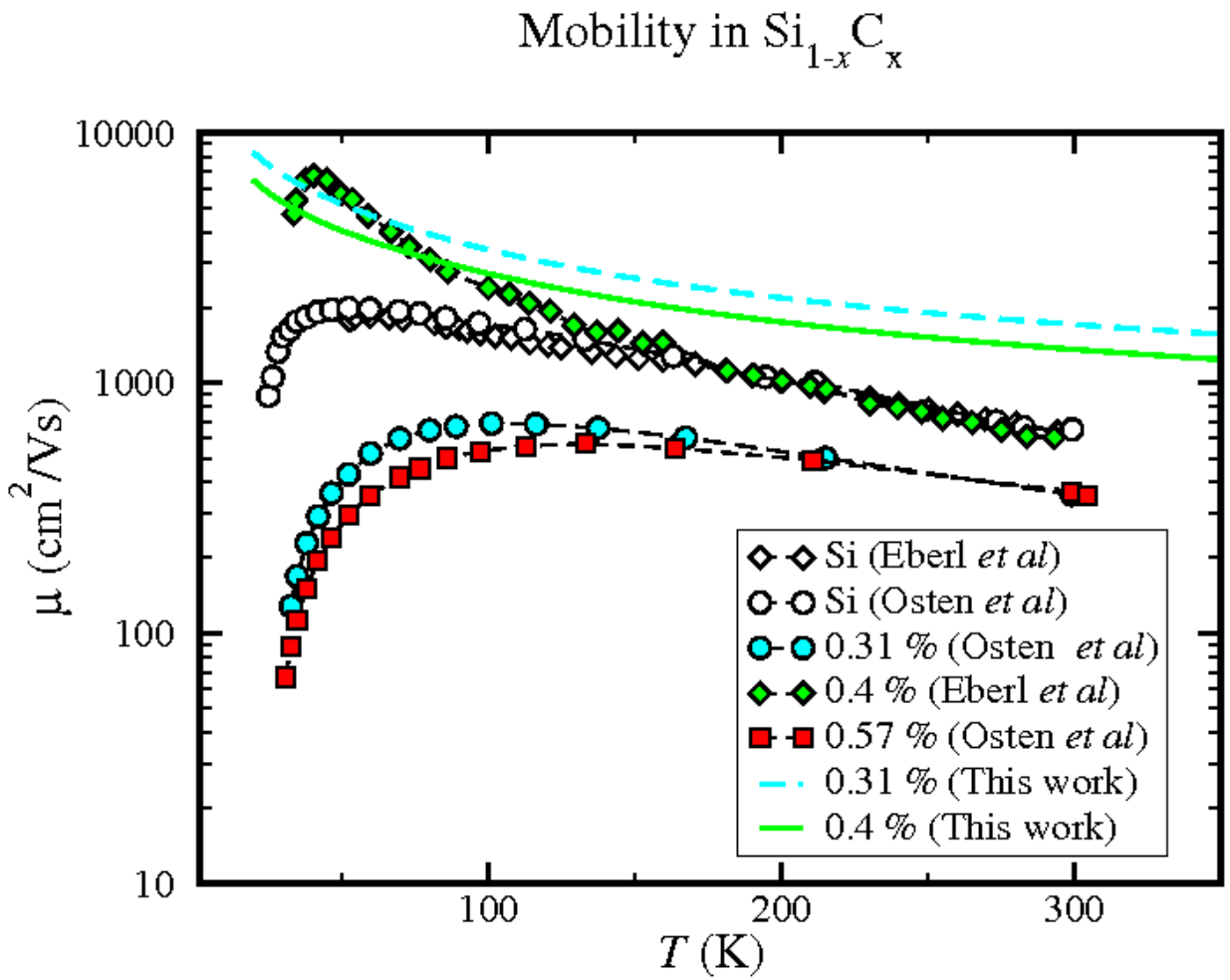


Scattering matrix calculations for 64 atom cell with C atom and with pure Si with the same ionic positions for each step in the relaxation algorithm.



***Intravalley*: 2.8 eV; *g-type*: 0.35 eV; *f-type* (not shown): 0.1 eV**

Mobility in Si(1-*x*)C(*x*)



Note: solid and dashed lines are calculated alloy scattering limited mobilities (no other scattering processes)

K Eberl, K Brunner and W Winter, Thin Solid Films, **294**, 98 (1997)
HJ Osten and P Gaworzewski, J. Appl. Phys., **82**, 4977 (1997)

- We can use DFT calculations as the basis for a model of carrier scattering
- The scattering matrix may be decomposed into two components due to chemical change and ionic relaxation
- For Si(1-*x*)C(*x*), intravalley scattering turns out to be the dominant process
- Scattering by substitutional C appears to be too weak to explain the observed degradation in mobility – conclude that this is due to interstitial defects

The first principles approach to alloy scattering:

F Murphy-Armando and S Fahy, Phys. Rev. Lett. **97**, 96606 (2006)

S Joyce, F Murphy-Armando, and S Fahy, Phys. Rev. B **75**, 155201 (2007)

F Murphy-Armando and S Fahy, Phys. Rev. B **78**, 35202 (2008)

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